UNCERTAINTY OF STABILITY VARIANCES BASED ON FINITE DIFFERENCES

C. A. Greenhall*

Jet Propulsion Laboratory

California Institute of Technology

W. J. Riley Symmetricom, Inc.

Abstract

This work gives an algorithm for computing the degrees of freedom of estimators of Allan and Hadamard variances, including their modified versions. A consistent approach is used throughout.

1 INTRODUCTION

This work gives an algorithm by which one can compute error bars for measurements of frequency stability variances in the presence of power-law phase noises. These stability variances fall into two categories: unmodified variances, which use dth differences of phase samples for d=2 (Allan) or 3 (Hadamard), and modified variances, which use dth differences of averaged phase samples. The corresponding sampling functions that act on phase and frequency are shown in [1]. Each variance is defined as a scaling factor times the expected value of the squared differences. Unbiased estimates of this variance are computed from available phase data by taking time averages of the squared differences. The usual choices for the estimation stride (the time step) are the sample period τ_0 and the averaging period τ , a multiple of τ_0 . These give, respectively, the overlapped estimator (OE) and nonoverlapped estimator (NOE) of the stability variance (although "nonoverlapped" is a misnomer; there is always some overlap between summands).

The new algorithm, which computes the equivalent degrees of freedom (edf) of a variance estimator, can replace several ones currently in use with a single, complete, and consistent method. Specifically, this algorithm covers the OE and NOE of the unmodified and modified Allan and Hadamard variances for all common noise types ($-4 \le \alpha \le 2$) at all applicable sample sizes and averaging factors. Previously, for the NOE of Allan and Hadamard variances, 1-sigma confidence limits were generally set by scaling the measured deviation by a noise-dependent factor K_{α}/\sqrt{M} , where M is the number of summands ([2-6]. For the OE of Allan variance, empirical edf approximations ([7-10]) were generally used along with chi-squared statistics; non-empirical methods for both Allan variance estimators were also published ([11-14]). Although an edf computation for the OE of

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Form Approved OMB No. 0704-0188 modified Allan (and time) variance was first given in [15], the simpler approach of [16] was generally used; an alternative unpublished approach using the Hadamard edf formed the basis of the new algorithm. As an example of the application of the new algorithm, the Stable32 program for frequency stability analysis [17] has adopted it (since Version 1.41) instead of the multiple algorithms previously used for setting confidence limits and error bars.

We wish to maintain a clear distinction between a stability variance and its estimators; in particular, we treat both the OE and the NOE of each variance. Even though the OE usually has lower uncertainty than the NOE, the NOE is convenient when phase data are processed in real time or read sequentially from a file. Indeed, the TSC 5110A Time Interval Analyzer [18], in its "averaging" mode, computes an NOE of modified Allan variance.

The goal of the new algorithm is not closed formulas, but fast numerical results whose accuracy is adequate for the purpose at hand. All the calculations are based on the same theoretical principles, with no empirical formulas. For each τ , one must choose a dominant phase-noise power law, $S_x(f) \sim Cf^{\alpha-2}$, where $\alpha \in \{2, 1, 0, -1, -2, -3, -4\}$ (white PM to random run FM); see [19] for a method of power-law identification. The phase noise is assumed to be approximately bandlimited to the Nyquist frequency $1/(2\tau_0)$.

Not covered are effects of trend removal, drift removal for Allan variance in particular; the dth phase differences are assumed to have zero mean. One can use Hadamard variance to obtain stability results that are invariant to linear frequency drift. Special long-term stability statistics, such as total Allan variance [20], total Hadamard variance [19], and Theo1 [21], are not covered; these require their own treatments.

2 THEORY OF OPERATION

Although the presentation of the algorithm is self-contained, we give a brief account of the theory behind it. The algorithm's output is the equivalent degrees of freedom (edf) of an unbiased estimator V of a stability variance $\sigma^2 = EV$. Define

$$\nu = \operatorname{edf} V = \frac{2(EV)^2}{\operatorname{var} V} = \frac{2\sigma^4}{\operatorname{var} V}.$$
(1)

It has been observed empirically (but not exhaustively) for these estimators that $(\nu/\sigma^2) V$ has approximately a χ^2_{ν} distribution. Thus, having computed ν and observed V, one can obtain confidence intervals of form $\nu V/x_2 \le \sigma^2 \le \nu V/x_1$ from χ^2_{ν} levels $x_1 < x_2$ [7].

The model for phase x(t) is the τ_0 -difference of a pure power-law process:

$$x\left(t\right) = \Delta_{\tau_0} w\left(t\right),\tag{2}$$

where w(t) is a continuous-time process with spectral density $Cf^{\alpha-4}$ for all f > 0, and Δ is the backward difference operator. Then $S_x(f)$ is asymptotically proportional to $f^{\alpha-2}$ as $f \to 0$ and has approximate bandwidth $1/(2\tau_0)$; this is the first reason for using w(t).

Now let

$$z\left(t\right) = \Delta_{\tau}^{d} \Delta_{\varepsilon} w\left(t\right),\tag{3}$$

where $\varepsilon = \tau_0$ or τ . For $\varepsilon = \tau_0$ we have $z(t) = \Delta_{\tau}^d x(t)$, which leads to an unmodified variance. For $\varepsilon = \tau = m\tau_0$ we observe from (2) that

$$\Delta_{\tau}w(t) = w(t) - w(t - m\tau_0) = \sum_{n=0}^{m-1} \Delta_{\tau_0}w(t - n\tau_0) = \sum_{n=0}^{m-1} x(t - n\tau_0) = m\bar{x}(t),$$

where $\bar{x}(t)$ is a discrete-time average of m samples of x. In this case, $z(t) = m\Delta_{\tau}^d \bar{x}(t)$, which leads to a modified variance [16]; this is the second reason for using w(t). In either case we assume that z(t) is a stationary zero-mean Gaussian process with autocovariance (ACV) function $s_z(t) = \operatorname{Ez}(u+t) z(u)$.

Ignoring the conventional scaling factors, we define the stability variance and its estimator by

$$\sigma^2 = Ez^2(t), V = \frac{1}{M} \sum_{n=1}^{M} z^2(n\delta),$$
 (4)

where the stride δ is τ_0 for the OE and τ for the NOE. The number of terms M depends on the estimator type and the number of data. We have $EV = \sigma^2 = s_z(0)$. Then $\text{cov}\left[z^2(t), z^2(u)\right] = 2s_z^2(u-t)$, and

$$\operatorname{var} V = \frac{2}{M^2} \sum_{n_1, n_2 = 1}^{M} s_z^2 \left((n_2 - n_1) \, \delta \right). \tag{5}$$

The definition (1), after substitution of (5), simplifies to

$$\frac{1}{\operatorname{edf} V} = \frac{1}{M} \left[1 + \frac{2}{s_z^2(0)} \sum_{j=1}^{M-1} \left(1 - \frac{j}{M} \right) s_z^2(j\delta) \right].$$
 (6)

The ACV $s_z(t)$ is obtained from (3) by applying a difference operator of order 2d + 2 to the generalized autocovariance (GACV) $s_w(t)$ of the power-law process w(t) [13,16]:

$$s_{z}(t) = (\Delta_{\tau} \Delta_{-\tau})^{d} \Delta_{\varepsilon} \Delta_{-\varepsilon} s_{w}(t).$$

The function $s_w(t)$ is given below for each α .

3 ALGORITHMS FOR EDF CALCULATION

Our purpose is to obtain practical numerical approximations of (6). We give two versions of the algorithm: the simplified version merely truncates the sum in the exact formula; the full version maintains the number of summation terms below a presassigned threshold and avoids catastrophic roundoff errors. They have the same inputs, output, function definitions, and initial step. Some explanation of the approximations is given in the Appendix. Because the results are invariant to time scaling, we may set $\tau = 1$, $\tau_0 = 1/m$.

All arithmetic is to be carried out in double-precision floating point. Operations that give signed integers are the floor function $\lfloor x \rfloor$ (greatest integer that is $\leq x$) and ceiling function $\lceil x \rceil = -\lfloor -x \rfloor$ (least integer that is $\geq x$).

3.1 Inputs

 α = frequency noise exponent

$$\alpha = 2, 1, 0, -1, -2, -3, -4$$

Noise type = WHPM, FLPM, WHFM, FLFM, RWFM, FWFM, RRFM

d =order of phase difference

d=1: first-difference variance (included for completeness)

d=2: Allanvariance

d=3: Hadamard variance

Restriction: $\alpha + 2d > 1$

 $m = \text{averaging factor } \tau/\tau_0, \text{ positive integer}$

F = filter factor

F = 1: modified variance

F = m: unmodified variance

 $S = \text{stride factor (estimator stride} = \tau/S)$

S=1: nonoverlapped estimator

S = m: overlapped estimator

N = number of phase data with sample period τ_0

3.2 Output

edf = equivalent degrees of freedom of the variance estimator

3.3 Constant and function definitions

Set an integer constant J_{max} (used only in the full version); we suggest $J_{\text{max}} = 100$.

The formal arguments of the following functions have the same names as the input arguments of the main algorithm.

1. Define the function $s_w(t, \alpha)$ as follows:

The entries with $\ln |t|$ must evaluate to 0 when t=0.

2. Define the function

$$s_{x}(t, F, \alpha) = F^{2} \Delta_{1/F} \Delta_{-1/F} s_{w}(t, \alpha)$$

$$= F^{2} \left[2s_{w}(t, \alpha) - s_{w} \left(t - \frac{1}{F}, \alpha \right) - s_{w} \left(t + \frac{1}{F}, \alpha \right) \right],$$

$$s_{x}(t, \infty, \alpha) = s_{w}(t, \alpha + 2), \quad -4 \le \alpha \le 0.$$
(8)

3. Define the function

$$s_z(t, F, \alpha, d) = (\Delta_1 \Delta_{-1})^d s_x(t, F, \alpha), \quad d = 1, 2, 3;$$
 (9)

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that is (with dependence on F and α suppressed on the right sides),

$$s_{z}(t, F, \alpha, 1) = 2s_{x}(t) - s_{x}(t-1) - s_{x}(t+1),$$

$$s_{z}(t, F, \alpha, 2) = 6s_{x}(t) - 4s_{x}(t-1) - 4s_{x}(t+1) + s_{x}(t-2) + s_{x}(t+2),$$

$$s_{z}(t, F, \alpha, 3) = 20s_{x}(t) - 15s_{x}(t-1) - 15s_{x}(t+1) + 6s_{x}(t-2) + 6s_{x}(t+2) - s_{x}(t-3) - s_{x}(t+3).$$

4. Define the function

BasicSum
$$(J, M, S, F, \alpha, d) = s_z^2(0, F, \alpha, d) + \left(1 - \frac{J}{M}\right) s_z^2 \left(\frac{J}{S}, F, \alpha, d\right)$$

 $+ 2\sum_{j=1}^{J-1} \left(1 - \frac{j}{M}\right) s_z^2 \left(\frac{j}{S}, F, \alpha, d\right).$ (10)

3.4 Initial steps for both versions

1. Compute M, the number of summands in the estimator, as follows:

$$L = \frac{m}{F} + md \quad \text{(an integer)},$$

$$M = 1 + \left| \frac{S(N - L)}{m} \right|$$
(11)

if $N \ge L$, otherwise there are not enough data. Remark: L is the length of the filter applied to the phase samples.

2. Let

$$J = \min\left(M, (d+1)S\right). \tag{12}$$

3.5 Main procedure, simplified version

This is just one step:

$$\frac{1}{\text{edf}} = \frac{1}{s_z^2(0, F, \alpha, d) M} \text{BasicSum}(J, M, S, F, \alpha, d).$$
(13)

To check the effect of the truncation, one can also try a larger value of J, say min (M, 6S).

3.6 Main procedure, full version

Let
$$r = \frac{M}{S}$$
.

There are four cases. The calculations use coefficients from three numerical tables.

3.6.1 Case 1. Modified variances: F = 1, all α

This case also applies to unmodified variances when F=m=1. If $J \leq J_{\text{max}}$

$$\frac{1}{\operatorname{edf}} = \frac{1}{s_z^2(0, 1, \alpha, d) M} \operatorname{BasicSum}(J, M, S, 1, \alpha, d)$$

Else if $J > J_{\text{max}}$ and $r \ge d + 1$, take a_0, a_1 from Table 1; then

$$\frac{1}{\text{edf}} = \frac{1}{r} \left(a_0 - \frac{a_1}{r} \right)$$

Else let $m' = \frac{J_{\text{max}}}{r}$ (not necessarily an integer); then

$$\frac{1}{\operatorname{edf}} = \frac{1}{s_z^2(0, 1, \alpha, d) J_{\max}} \operatorname{BasicSum} \left(J_{\max}, J_{\max}, m', 1, \alpha, d\right)$$

3.6.2 Case 2. Unmodified variances, WHFM to RRFM: F = m, $\alpha \leq 0$

If $J \leq J_{\text{max}}$

If $m(d+1) \leq J_{\text{max}}$ then let m' = m else let $m' = \infty$. Then

$$\frac{1}{\operatorname{edf}} = \frac{1}{s_z^2(0, m', \alpha, d) M} \operatorname{BasicSum} (J, M, S, m', \alpha, d)$$

Else if $J > J_{\text{max}}$ and $r \ge d + 1$, take a_0, a_1 from Table 2; then

$$\frac{1}{\text{edf}} = \frac{1}{r} \left(a_0 - \frac{a_1}{r} \right)$$

Else let $m' = \frac{J_{\text{max}}}{r}$ (not necessarily an integer); then

$$\frac{1}{\operatorname{edf}} = \frac{1}{s_z^2(0, \infty, \alpha, d) J_{\max}} \operatorname{BasicSum} \left(J_{\max}, J_{\max}, m', \infty, \alpha, d\right)$$

3.6.3 Case 3. Unmodified variances, FLPM: F = m, $\alpha = 1$

If $J \leq J_{\text{max}}$

$$\frac{1}{\mathrm{edf}} = \frac{1}{s_z^2\left(0,m,1,d\right)M} \mathrm{BasicSum}\left(J,M,S,m,1,d\right).$$

Remark: For this case, m must be less than about 10^6 to avoid roundoff error. Else if $J > J_{\text{max}}$ and $r \ge d+1$, take a_0, a_1 from Table 2 ($\alpha = 1$), b_0, b_1 from Table 3; then

$$\frac{1}{\text{edf}} = \frac{1}{(b_0 + b_1 \ln m)^2 r} \left(a_0 - \frac{a_1}{r} \right)$$

Else let $m' = \frac{J_{\text{max}}}{r}$ (not necessarily an integer); then

$$\frac{1}{\operatorname{edf}} = \frac{1}{(b_0 + b_1 \ln m)^2 J_{\max}} \operatorname{BasicSum} (J_{\max}, J_{\max}, m', m', 1, d)$$

3.6.4 Case 4. Unmodified variances, WHPM: $F=m, \ \alpha=2$

This calculation is exact, and can be expressed in closed form. In these formulas, $\binom{n}{k}$ denotes the binomial coefficient $\frac{n!}{k!\,(n-k)!}$. Let $K=\lceil r \rceil$. If $K \leq d$

$$\frac{1}{\text{edf}} = \frac{1}{M} \left[1 + \frac{2}{\binom{2d}{d}} \sum_{k=1}^{K-1} \left(1 - \frac{k}{r} \right) \left(\frac{2d}{d-k} \right)^2 \right]$$

Else

$$\frac{1}{\text{edf}} = \frac{1}{M} \left(a_0 - \frac{a_1}{r} \right),$$

where

$$a_0 = \frac{\binom{4d}{2d}}{\binom{2d}{d}^2}, \quad a_1 = \frac{d}{2},$$

also given in Table 2 ($\alpha = 2$).

3.7 Tables

Table 1. Coefficients for modified variances.

| | d = 1 | | d = 2 | | d = 3 | |
|----------|---------------|---------------|---------------|--------------------|-----------------|---------------|
| α | a_0 | a_1 | a_0 | a_1 | a_0 | a_1 |
| 2 | $\frac{2}{3}$ | $\frac{1}{3}$ | $\frac{7}{9}$ | $\frac{1}{2}$ | $\frac{22}{25}$ | $\frac{2}{3}$ |
| 1 | 0.840 | 0.345 | 0.997 | $0.\overline{6}16$ | | 0.843 |
| 0 | 1.079 | 0.368 | 1.033 | 0.607 | 1.184 | 0.848 |
| -1 | | | 1.048 | 0.534 | 1.180 | 0.816 |
| -2 | | | 1.302 | 0.535 | 1.175 | 0.777 |
| -3 | | | | | 1.194 | 0.703 |
| -4 | | | | | 1.489 | 0.702 |

Table 2. Coefficients for unmodified variances.

| | d = 1 | | d = 2 | | d = 3 | |
|----------|---------------|---------------|-----------------|---------------|-------------------|---------------------|
| α | a_0 | a_1 | a_0 | a_1 | a_0 | a_1 |
| 2 | $\frac{3}{2}$ | $\frac{1}{2}$ | $\frac{35}{18}$ | 1 | $\frac{231}{100}$ | $\frac{3}{2}$ |
| 1 | 78.6 | 25.2 | 790. | 410. | 9950. | $65\overline{20}$. |
| 0 | $\frac{2}{3}$ | $\frac{1}{6}$ | $\frac{2}{3}$ | $\frac{1}{3}$ | $\frac{7}{9}$ | $\frac{1}{2}$ |
| -1 | | | 0.852 | 0.375 | 0.997 | $0.\overline{6}17$ |
| -2 | | | 1.079 | 0.368 | 1.033 | 0.607 |
| -3 | | | | | 1.053 | 0.553 |
| -4 | | | | | 1.302 | 0.535 |

Table 3. Coefficients for logarithmic denominator, unmodified variances, FLFM ($\alpha = 1$).

4 EXAMPLES

First, we must point out that the new edf values differ somewhat from older ones because of our choice of phase noise model. Previously (for $\alpha < -1$) the phase was generally assumed to have a pure $f^{\alpha-2}$ spectrum; here, the phase is modeled as the first difference of an $f^{\alpha-4}$ process. For example, consider overlapped Allan variance, white FM, 1025 phase data. The old results are from [14] (close to those of [7].

$$\tau/\tau_0$$
 1 2 4 8 16 32 64 128 256 512 old edf 682 584 354 186.3 93.4 45.8 21.8 9.83 4.01 1 new edf 801 554 314 170.0 88.5 44.4 21.8 9.83 4.00 1

The old and new results are in practical agreement at the larger values of τ , where the results matter more. By allowing this mild discrepancy, we were able to make the algorithm simpler and more uniform.

Figures 1 and 2 (at the end of the paper) show examples of edf, computed by the new algorithm, as a function of noise type and of variance type with other parameters fixed.

5 CONCLUSION

The stability variances considered here can all be put into the same form, namely, the mean-square average of the output of a finite-difference filter acting, not on the phase samples, but on their cumulative sums. With this insight, we have been able to make an algorithm for computing the equivalent degrees of freedom of variance measurements. It covers all the commonly used variances and estimators, and then some. There is now a single unified source for these uncertainty calculations instead of the many papers that each cover only one variance and perhaps only one estimator of it. Complete pseudocode for the new algorithm is given here; software is available on request [23].

6 APPENDIX: EXPLANATIONS OF APPROXIMATIONS

As is, (6) is unfit for numerical computation. We find empirically that $s_z^2(t)$ tends rapidly to zero as t increases beyond d. For the accuracy needed here (a few percent), there is no point in allowing j/S to be more than d+1. Indeed, for sufficiently large t the calculation of $s_z^2(t)$ blows up from roundoff error, even in double precision, because linear combinations of large s_w values are taken to get small s_z values. At the very least, one should truncate the sum at j = (d+1)S, as in the simplified version of the algorithm.

The full version of the algorithm uses the following general strategy. If $J \leq J_{\text{max}}$ we do the summation (6). When $J > J_{\text{max}}$ there are two cases. First, if $M \geq (d+1)S$ then $S = m \geq J_{\text{max}}/(d+1) >> 1$. We truncate the sum at (d+1)S and approximate it by an integral; this gives

$$\frac{1}{\operatorname{edf} V_d} \approx \frac{2}{r} \int_0^{d+1} \left(1 - \frac{t}{r} \right) s_z^2(t) dt$$
$$= \frac{1}{r} \left(a_0 - \frac{a_1}{r} \right),$$

where

$$r = \frac{M}{S}$$
, $a_0 = 2 \int_0^{d+1} s_z^2(t) dt$, $a_1 = 2 \int_0^{d+1} s_z^2(t) t dt$.

These coefficients can be evaluated in advance. Second, if M < (d+1)S then we do another summation in which J is reduced from M to J_{max} and S is reduced proportionately from m.

The extra term for j = J in BasicSum makes the sum a trapezoidal approximation to the integral, whether or not the sum is truncated.

This method works straightforwardly for Case 1; indeed, in this setting the modified variances are simpler than the unmodified ones. In Case 2, when m is large we compute $s_z(t)$ using the limiting form $s_x(t,\infty)$, which is actually $-s''_w(t)$. This means that we are treating x(t) as w'(t), the process w(t) being differentiable in the mean-square sense.

The most troublesome case is the overlapped estimators of the unmodified variances for flicker PM. As $S = m \to \infty$, $s_z(t)$ approaches a function with logarithmic singularities. The factor $b_0 + b_1 \ln m$ is an asymptotic form of $s_z(0)$. It would be possible (though inconvenient) to add another large-m subcase as in Case 2, but one does not expect flicker PM to be the dominant noise type when m is large.

Case 4 is constructed by knowing that the phase samples are accurately uncorrelated when w(t) is a Wiener process. The simplified computation (13) is correct, but wasteful, because $s_z(t)$ is a linear combination of hat-shaped peaks of width 2/m.

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- [23] Upon request by e-mail to edf@wriley.com, the second author will send an electronic copy of C source code that implements this algorithm, along with a small Microsoft Windows (r) program that computes the edf for various cases.

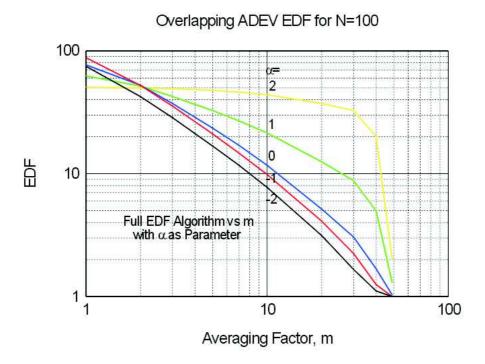


Figure 1. Edf vs. averaging factor with power-law noise type as a parameter: Allan variance, overlapped estimator, 100 phase samples.

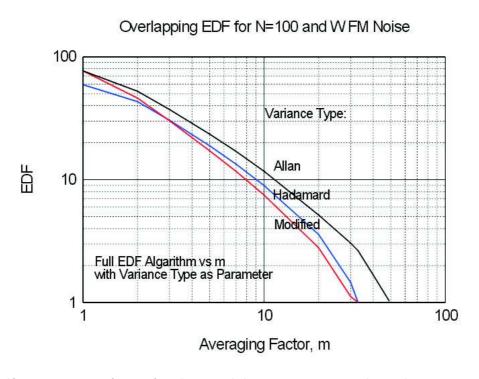


Figure 2. Edf vs. averaging factor for three stability variances: overlapped estimator, white FM, 100 phase samples.

QUESTIONS AND ANSWERS

DON PERCIVAL (University of Washington): Your algorithm, your recipe handles the integer power laws. How hard would it be to include something like the power law of minus five-thirds, which would make people in the atmospheric turbulence community very happy.

CHUCK GREENHALL: It would not be difficult to do a specific extra power. It would be more work to include a whole continuous range. The algorithm is split up into four cases for purposes of numerical computation. So it would be a modest computation.

MARC WEISS (National Institute of Standards and Technology): I guess I missed it, but it sounds like you need to know the power law before you can get the confidence.

GREENHALL: That is correct.

WEISS: So how do you suggest doing that?

GREENHALL: Well, a couple years ago there was a paper in which both of us were co-authors, and it actually published the method being in the Stable software. Bill and I have a paper coming up at EFTF in which we have developed a simpler and better method involving the lag-1 autocorrelation.

DEMETRIOS MATSAKIS (U.S. Naval Observatory): Maybe a better way to phrase the other question was: what percentage of the error is due to the error bars? You have a certain contribution because you do not know how to fit your power law. So how much does it raise your error?

GREENHALL: Well, I don't know. We were pulling ourselves up by our bootstraps here, and you're probably most conservative to assume the more red power law if you are uncertain about it. That is the best thing I can say.

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